



Ames' Bakac
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chemistry
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Research Highlights . . .

A better Lyme disease vaccine

Spring has finally arrived, but, unfortunately, the season often brings an abundance of deer ticks, which spread Lyme disease. The potentially debilitating illness is the most common vector-borne disease in the U.S. The current vaccine for the disease is based on OspA, an outer surface protein of the Lyme disease bacterium. The protein's structure was deciphered at [Brookhaven National Laboratory](#). Recently, a Brookhaven research team has determined the three-dimensional structure of OspC, another key protein of the Lyme disease bacterium. This research may lead to a second-generation vaccine that would be more effective than the current one.

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Microprobe expands X-ray capabilities

Conventional X-ray techniques have profoundly affected our lives. The benefits of X-ray research include advanced materials, new drug designs, and more accurate medical diagnostic methods. All those benefits may increase a thousand times with the superior resolution of the hard X-ray scanning microprobe, developed at the Advanced Photon Source at DOE's [Argonne National Laboratory](#). The microprobe offers unprecedented capabilities for imaging, which open many exciting new applications in microelectronics and in materials, biomedical, and environmental sciences. The microprobe provides high penetration power, allowing studies to be performed in vacuum or in ambient pressure, or even in an aqueous environment, with applications to a broad range of samples and configurations.

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Ames investigates new superconductor

Researchers at the DOE's [Ames Laboratory](#) are gaining a better understanding of the physics operating in a remarkable new superconducting compound. The compound, magnesium diboride, becomes superconducting at 39 Kelvin (-389 F), nearly twice the temperature of intermetallic superconductors currently in use. In addition to addressing the mechanism of superconductivity in magnesium diboride, the Ames Lab researchers have gone on to map the compound's properties and create wire segments of the material, all in one month's time.

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Tevatron begins Collider Run II

Batavia, Ill-Officials at DOE's [Fermi National Accelerator Laboratory](#) announced the March 1, 2001 start of Collider Run II at the Tevatron, the highest-energy particle accelerator now operating in the world. Researchers at Fermilab hope that high-energy particle collisions at the Tevatron in Run II will yield significant, long-awaited discoveries about the fundamental nature of matter in the universe. World attention has focused on Fermilab's two collider detectors at the Tevatron, CDF and DZero, as the next possible venue for discovery of the Higgs boson, an as-yet-unseen particle that physicists believe may determine the property of mass.

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DOE Pulse highlights work being done at the [Department of Energy's](#) national laboratories. [DOE's laboratories](#) house world-class facilities where more than 30,000 scientists and engineers perform cutting-edge research spanning DOE's science, energy, national security and environmental quality missions. *DOE Pulse* (www.ornl.gov/news/pulse/) is distributed every two weeks. For more information, please contact Jeff Sherwood (jeff.sherwood@hq.doe.gov, 202-586-5806).

Jlab lends superconducting skill to SNS mix

DOE's [Jefferson Lab](#) is lending its expertise in superconducting linear accelerator technology to DOE's construction of the [Spallation Neutron Source](#), which will be, when completed around 2006, the world's leading major neutron research facility.



Artist's concept of the SNS

Jefferson Lab last year joined a partnership of DOE's national laboratories including Argonne, Brookhaven, Lawrence Berkeley, Los Alamos and Oak Ridge to assist in the design, engineering and construction of the \$1.4 billion SNS in Oak Ridge, Tenn. The SNS will provide the most intense pulsed-neutron beams in the world for scientific research and industrial development.

The SNS will produce short, powerful proton pulses that will strike a liquid mercury target to produce neutrons through a process known as spallation. Neutrons freed by spallation will be slowed down in a device known as a moderator and guided through beam lines to areas containing specialized neutron detectors and other experimental devices. Once distributed, neutrons of different energies can be used in a wide variety of experiments.

Jefferson Lab's expertise in superconducting radio frequency (SRF) techniques and advanced accelerating components is being incorporated into the SNS design to enable low-cost, high efficiency accelerator operations. Jefferson Lab is engineering assembling most of the SNS accelerating components in Newport News, Va., and will oversee the installation of a helium refrigeration plant and an SRF facility at Oak Ridge.

JLab is joining the SNS effort with Lawrence Berkeley, responsible for designing and building the SNS' front-end system. Los Alamos is responsible for the SNS linear accelerator, which will speed up a negative hydrogen ion beam from 2.5 million electron volts to 1 billion electron volts. Brookhaven is designing and building a device called the accumulator ring structure, which bunches and intensifies the ion beam for delivery onto the mercury target to produce the pulsed neutron beams. Oak Ridge National Laboratory is responsible for target design and construction while Argonne develops the neutron-scattering instrumentation for the SNS works closely with ORNL to develop the experiment facilities.

The six-lab collaboration has been hailed as a key to the successful funding, design and completion of the SNS, and could serve as a model for large and complex science facilities of the future.

Submitted by DOE's [Jefferson Lab](#)

FROM CLASSICS TO CHEMISTRY

Andreja Bakac is a senior chemist at DOE's [Ames Laboratory](#). She grew up in Croatia and might easily have become a professor of comparative literature were it not for a remark made by her high school chemistry teacher.



Andreja Bakac

"He said, 'Girls belong in the kitchen, not in the lab,'" says Bakac. "He didn't mean to offend anybody, but I took that comment as a challenge."

Although literature and languages fascinated Bakac, she chose a different career path. "Chemistry was the very next thing I loved, and I've never regretted that choice."

Bakac's research focuses on fundamental chemistry, because, as she says, "nothing happens without it." She specializes in oxidation reactions and has successfully used visible light and oxygen to photooxidize hydrocarbons to industrially important chemicals. However, her current work involves thermal oxidation and using metals to drive different chemical reactions.

"Instead of using light to activate the substrate, I'm now using transition metal complexes to activate the oxygen," she explains. "These metals bind to and partially reduce molecular oxygen, making it more reactive to a variety of substrates."

Bakac is particularly interested in the intermediates, or precursors to desired products, resulting from her thermal oxidation experiments. "We capture them and explore their chemistry," she says. "Then we compare our metal-based intermediates with those derived from organic materials in the presence of molecular oxygen. There's a lot of similarity, but there's also much that is different and surprising."

Bakac explains that transition metals have a number of electronic levels and oxidation states that generate many intermediates not available in organic chemistry. "We've seen a lot of intermediates, which is exciting, and we've generated some of them independently," she says. "Now, we're beginning to understand the mechanism by which transition metal complexes catalyze oxidations of organic materials with molecular oxygen."

Submitted by DOE's [Ames Laboratory](#)